Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 04:37 AM EDT

PDB ID	:	3LMY
Title	:	The Crystal Structure of beta-hexosaminidase B in complex with Pyrimethamine
Authors	:	Bateman, K.S.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.; Tropak, M.; James, M.N.G.
Deposited on	:	2010-02-01
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

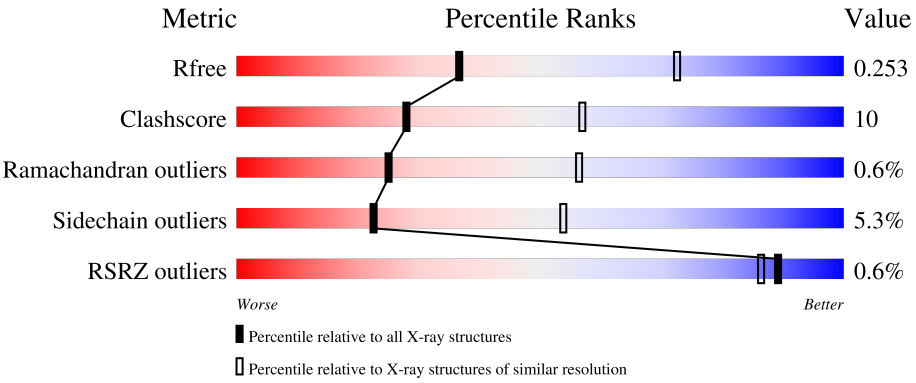
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	% 67% 17% · 14%
1	B	556	% 63% 22% · 14%
2	C	3	100%
3	D	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	561	-	-	-	X
6	CP6	A	562	-	-	X	-
6	CP6	B	563	-	-	X	-

2 Entry composition (i)

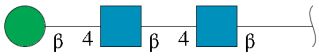
There are 8 unique types of molecules in this entry. The entry contains 8004 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3873	2503	642	715	13			
1	B	480	Total	C	N	O	S	0	0	0
			3877	2505	643	716	13			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

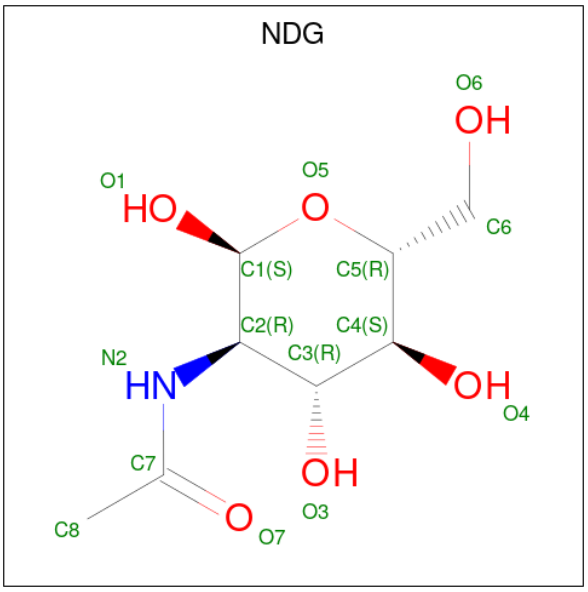


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

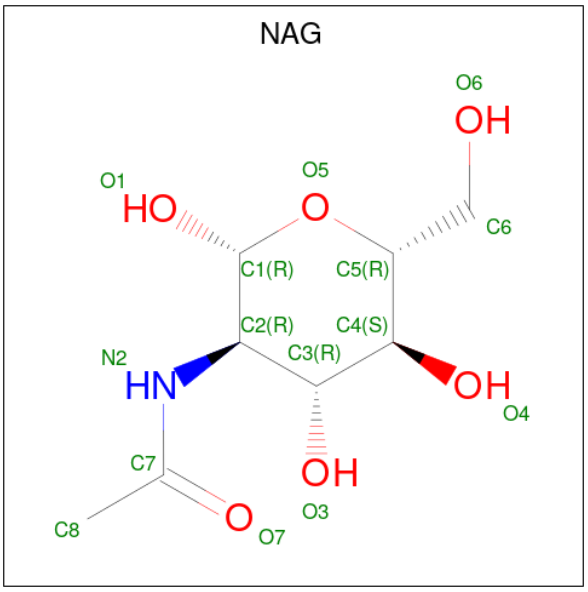
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0

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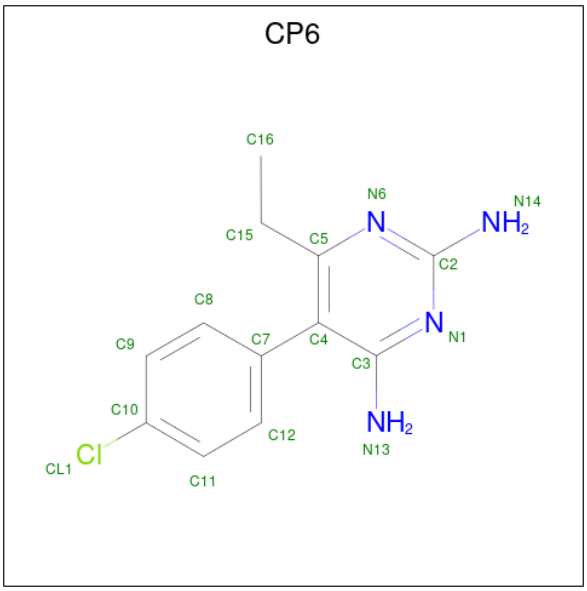
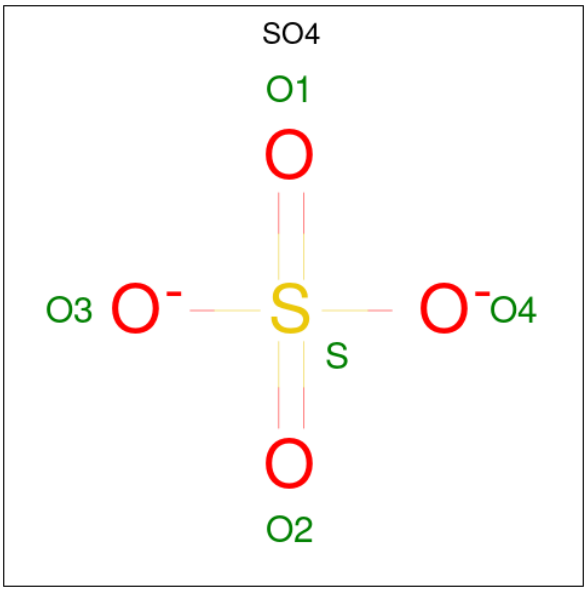
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 5-(4-CHLORO-PHENYL)-6-ETHYL-PYRIMIDINE-2,4-DIAMINE (three-letter code: CP6) (formula: $C_{12}H_{13}ClN_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Cl N 17 12 1 4	0	0
6	B	1	Total C Cl N 17 12 1 4	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

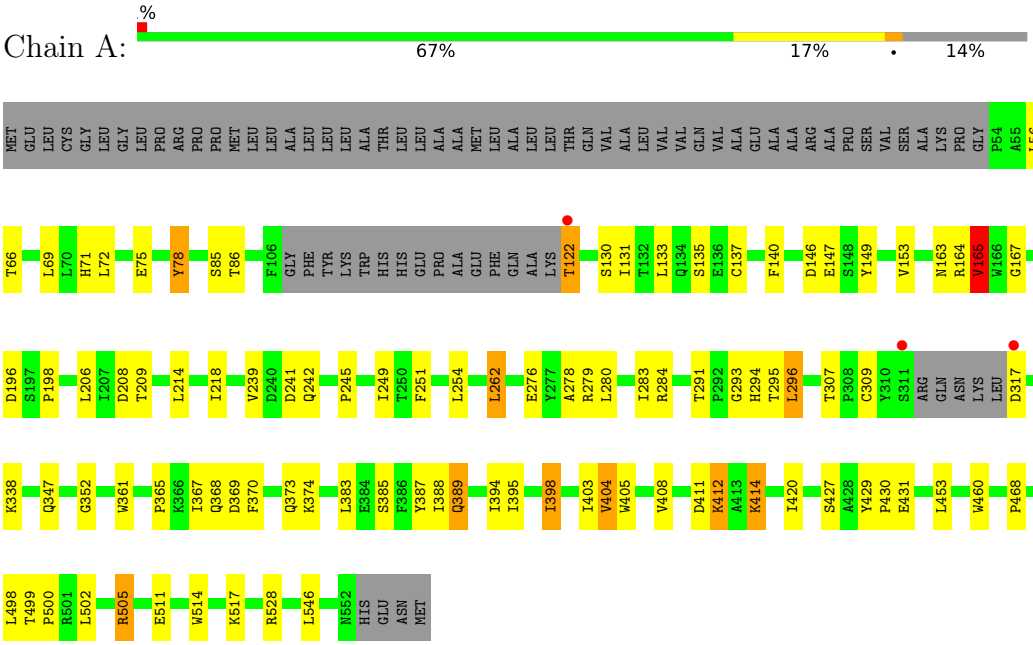
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	43	Total O 43 43	0	0
8	B	35	Total O 35 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

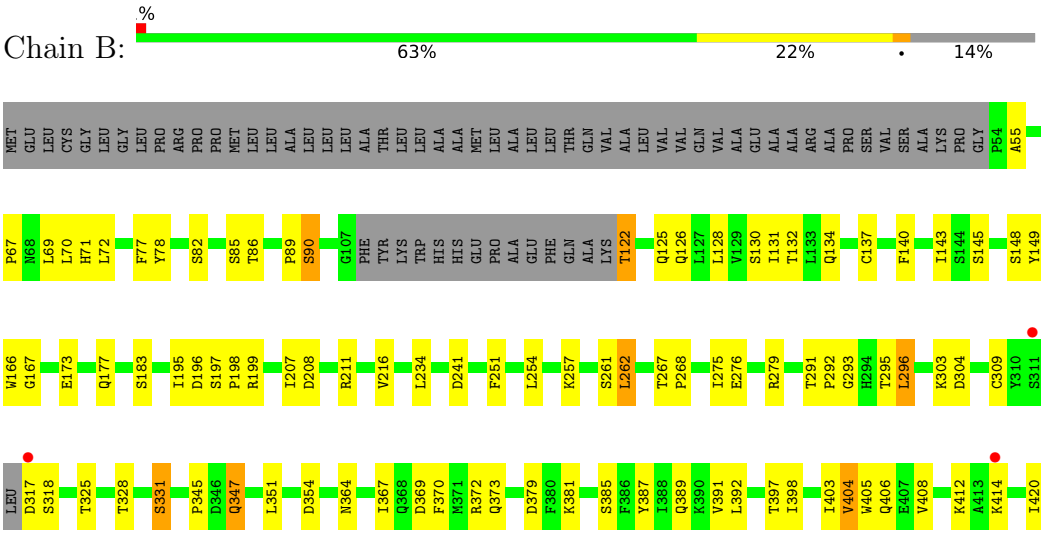
• Molecule 1: Beta-hexosaminidase subunit beta

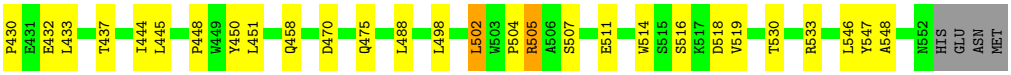
Chain A:



• Molecule 1: Beta-hexosaminidase subunit beta

Chain B:





• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	113.90Å 113.90Å 397.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.90 – 2.80 35.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (35.90-2.80) 92.2 (35.89-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.194 , 0.252 0.204 , 0.253	Depositor DCC
R_{free} test set	1801 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8004	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CP6, NAG, NDG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.86	2/3984 (0.1%)	0.88	5/5418 (0.1%)
1	B	0.79	0/3988	0.86	4/5423 (0.1%)
All	All	0.83	2/7972 (0.0%)	0.87	9/10841 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	CG-CD	5.58	1.60	1.51
1	A	487	CYS	CB-SG	-5.09	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	137	CYS	CB-CA-C	-5.67	99.06	110.40
1	B	137	CYS	CB-CA-C	-5.64	99.12	110.40
1	B	505	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	284	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	199	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	199	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	208	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	262	LEU	CB-CG-CD1	5.03	119.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3873	0	3778	61	0
1	B	3877	0	3780	88	0
2	C	39	0	34	4	0
3	D	28	0	25	2	0
4	A	14	0	12	0	0
4	B	14	0	12	0	0
5	A	14	0	13	0	0
5	B	28	0	26	0	0
6	A	17	0	13	8	0
6	B	17	0	13	7	0
7	B	5	0	0	0	0
8	A	43	0	0	1	0
8	B	35	0	0	2	0
All	All	8004	0	7706	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:TYR:CE2	6:B:563:CP6:H9	2.01	0.95
1:B:450:TYR:CD2	6:B:563:CP6:H9	2.06	0.91
1:B:351:LEU:HD13	1:B:391:VAL:HG12	1.55	0.84
6:A:562:CP6:H132	6:A:562:CP6:H8	1.40	0.83
6:A:562:CP6:H132	6:A:562:CP6:C8	1.96	0.79
1:A:389:GLN:NE2	1:A:414:LYS:HB3	1.99	0.78
1:A:198:PRO:HG3	1:A:514:TRP:CZ3	2.18	0.77
1:B:55:ALA:HA	8:B:593:HOH:O	1.85	0.74
1:B:389:GLN:HE22	1:B:414:LYS:HB3	1.53	0.73
6:A:562:CP6:H8	6:A:562:CP6:N13	2.02	0.72
1:B:450:TYR:CE2	6:B:563:CP6:C9	2.72	0.71
1:B:450:TYR:HE2	6:B:563:CP6:C9	2.04	0.71
1:A:403:ILE:HG12	1:A:420:ILE:HB	1.72	0.70
1:B:369:ASP:OD1	1:B:372:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:CE1	1:A:279:ARG:HD3	2.30	0.67
1:A:135:SER:O	1:A:165:VAL:HB	1.96	0.66
1:A:352:GLY:HA2	1:A:405:TRP:CD1	2.30	0.66
1:B:450:TYR:HE2	6:B:563:CP6:C8	2.11	0.64
1:A:65:MET:HE2	2:C:1:NAG:H82	1.80	0.63
1:B:530:THR:CG2	1:B:546:LEU:HD12	2.28	0.63
1:A:370:PHE:CZ	1:A:374:LYS:HE3	2.34	0.62
1:A:369:ASP:O	1:A:373:GLN:HG3	2.00	0.61
1:B:351:LEU:HD12	1:B:392:LEU:HD23	1.82	0.61
1:A:404:VAL:HG13	1:A:408:VAL:HB	1.82	0.60
6:A:562:CP6:C8	6:A:562:CP6:N13	2.61	0.59
1:B:149:TYR:CE1	1:B:196:ASP:HB3	2.36	0.59
1:B:150:THR:HG22	1:B:195:ILE:HG12	1.84	0.59
1:A:69:LEU:O	1:A:122:THR:HG22	2.04	0.58
1:B:293:GLY:O	1:B:295:THR:HG23	2.04	0.58
1:B:369:ASP:O	1:B:373:GLN:HG3	2.03	0.58
1:A:86:THR:HG23	1:A:131:ILE:O	2.04	0.57
1:A:389:GLN:HE22	1:A:414:LYS:HB3	1.66	0.57
1:A:206:LEU:C	1:A:206:LEU:HD23	2.25	0.57
1:B:379:ASP:OD1	1:B:381:LYS:HB2	2.05	0.57
1:B:71:HIS:N	1:B:122:THR:O	2.36	0.56
1:A:69:LEU:HD21	2:C:1:NAG:H62	1.88	0.56
1:A:370:PHE:HA	1:A:373:GLN:OE1	2.06	0.56
1:A:498:LEU:C	1:A:498:LEU:HD23	2.26	0.56
1:B:347:GLN:HA	1:B:347:GLN:OE1	2.06	0.55
1:B:173:GLU:O	1:B:177:GLN:HG3	2.05	0.55
1:B:404:VAL:HG13	1:B:408:VAL:HB	1.88	0.55
1:B:291:THR:HB	1:B:387:TYR:OH	2.07	0.54
1:A:153:VAL:HG11	1:A:189:ILE:HG12	1.89	0.54
1:B:140:PHE:CE1	1:B:279:ARG:HD3	2.42	0.54
1:A:241:ASP:OD1	1:A:296:LEU:HB2	2.08	0.54
1:A:404:VAL:CG1	1:A:408:VAL:HB	2.38	0.54
1:B:78:TYR:CD1	1:B:78:TYR:N	2.75	0.54
1:A:429:TYR:N	1:A:430:PRO:CD	2.71	0.54
1:A:499:THR:HB	1:A:500:PRO:CD	2.39	0.53
1:A:324:PRO:HG2	1:A:383:LEU:HD11	1.90	0.53
1:B:351:LEU:HD13	1:B:391:VAL:CG1	2.35	0.53
1:B:406:GLN:NE2	1:B:432:GLU:HG3	2.23	0.53
1:B:145:SER:HB3	1:B:166:TRP:CD1	2.43	0.53
1:B:291:THR:HG22	1:B:295:THR:HG21	1.91	0.53
1:A:293:GLY:O	1:A:295:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASP:OD2	1:B:211:ARG:HD3	2.08	0.53
6:A:562:CP6:H152	6:A:562:CP6:C12	2.39	0.53
1:B:403:ILE:HG12	1:B:420:ILE:HB	1.92	0.52
1:B:89:PRO:HD2	8:B:574:HOH:O	2.09	0.52
1:B:530:THR:HG22	1:B:546:LEU:HD12	1.89	0.52
1:A:71:HIS:C	1:A:72:LEU:HD12	2.30	0.52
1:A:309:CYS:HB2	1:A:317:ASP:O	2.09	0.52
1:B:389:GLN:NE2	1:B:414:LYS:HB3	2.24	0.52
1:B:445:LEU:HD11	1:B:448:PRO:HD3	1.92	0.52
1:B:85:SER:HB2	1:B:130:SER:HA	1.91	0.52
1:B:69:LEU:O	1:B:122:THR:HG22	2.10	0.52
1:B:328:THR:O	1:B:331:SER:HB2	2.11	0.51
2:C:2:NAG:H62	2:C:3:BMA:H2	1.92	0.51
1:B:150:THR:CG2	1:B:195:ILE:HG12	2.41	0.51
1:B:267:THR:HB	1:B:268:PRO:HD2	1.92	0.51
1:A:56:LEU:O	1:A:528:ARG:NH1	2.43	0.51
1:B:516:SER:HB2	1:B:519:VAL:HG23	1.92	0.51
1:B:354:ASP:HB3	1:B:405:TRP:CD1	2.46	0.50
1:A:239:VAL:HG12	1:A:245:PRO:HD2	1.92	0.50
1:B:65:MET:HE2	3:D:1:NAG:H82	1.93	0.50
1:B:86:THR:HG23	1:B:131:ILE:O	2.11	0.50
6:A:562:CP6:H152	6:A:562:CP6:H12	1.93	0.50
6:A:562:CP6:C15	6:A:562:CP6:H12	2.42	0.50
1:A:293:GLY:O	1:A:294:HIS:HB2	2.11	0.50
1:B:82:SER:HB3	1:B:128:LEU:HB3	1.93	0.50
1:B:404:VAL:CG1	1:B:408:VAL:HB	2.42	0.50
1:A:403:ILE:HG22	1:A:404:VAL:N	2.27	0.50
1:A:58:PRO:HB3	1:A:511:GLU:HA	1.94	0.49
1:B:58:PRO:HB3	1:B:511:GLU:HA	1.93	0.49
1:A:453:LEU:HD21	6:A:562:CP6:CL1	2.49	0.49
1:B:530:THR:HG23	1:B:546:LEU:HD12	1.94	0.49
1:B:309:CYS:HB2	1:B:317:ASP:O	2.12	0.49
1:A:249:ILE:HG21	1:B:90:SER:HB3	1.94	0.49
1:A:85:SER:HB2	1:A:130:SER:HA	1.95	0.49
1:B:143:ILE:O	1:B:143:ILE:HG13	2.13	0.48
1:A:78:TYR:CD1	1:B:262:LEU:HD21	2.48	0.48
1:B:82:SER:HA	1:B:128:LEU:HD22	1.95	0.48
1:B:67:PRO:O	3:D:1:NAG:H62	2.14	0.48
1:A:146:ASP:HB3	1:A:164:ARG:HG3	1.95	0.48
1:B:450:TYR:HD2	6:B:563:CP6:H9	1.72	0.48
1:A:72:LEU:HD12	1:A:72:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HA	1:B:122:THR:HG22	1.96	0.47
1:B:149:TYR:CZ	1:B:196:ASP:HB3	2.50	0.47
1:B:429:TYR:N	1:B:430:PRO:CD	2.77	0.47
1:A:149:TYR:CZ	1:A:196:ASP:HB3	2.50	0.47
1:A:411:ASP:HA	1:A:412:LYS:HE3	1.97	0.46
1:B:488:LEU:HD22	1:B:502:LEU:HG	1.97	0.46
1:B:518:ASP:OD1	1:B:518:ASP:N	2.41	0.46
1:B:351:LEU:CD1	1:B:392:LEU:HD23	2.44	0.46
1:B:303:LYS:O	1:B:304:ASP:HB2	2.13	0.46
1:A:65:MET:CE	2:C:1:NAG:H82	2.44	0.46
1:B:450:TYR:HE2	6:B:563:CP6:H8	1.80	0.46
1:A:505:ARG:HG3	8:A:587:HOH:O	2.14	0.45
1:A:251:PHE:HB2	1:A:254:LEU:HD12	1.99	0.45
1:A:209:THR:HG22	1:A:214:LEU:HB2	1.99	0.45
1:B:72:LEU:HD12	1:B:72:LEU:N	2.32	0.45
1:B:347:GLN:OE1	1:B:347:GLN:CA	2.65	0.45
1:A:395:ILE:HA	1:A:398:ILE:HD11	1.98	0.45
1:A:468:PRO:HB3	1:A:481:PHE:CZ	2.52	0.44
1:B:351:LEU:CD1	1:B:391:VAL:HG12	2.39	0.44
1:B:406:GLN:HE22	1:B:432:GLU:HG3	1.82	0.44
1:B:451:LEU:O	1:B:505:ARG:NH2	2.47	0.44
1:B:69:LEU:O	1:B:122:THR:CG2	2.66	0.44
1:B:77:PHE:C	1:B:78:TYR:HD1	2.21	0.44
1:B:292:PRO:HB3	1:B:387:TYR:CE2	2.53	0.44
1:A:78:TYR:CD1	1:A:78:TYR:N	2.83	0.44
1:A:361:TRP:CD1	1:A:367:ILE:HD13	2.53	0.44
1:A:365:PRO:O	1:A:368:GLN:HB2	2.17	0.44
1:A:394:ILE:O	1:A:398:ILE:HD13	2.18	0.44
1:B:241:ASP:OD1	1:B:296:LEU:HB2	2.18	0.44
1:B:516:SER:HB3	1:B:518:ASP:OD1	2.18	0.43
1:B:197:SER:HB2	1:B:198:PRO:HD2	2.00	0.43
1:A:133:LEU:HD12	1:A:163:ASN:HB3	2.01	0.43
1:B:351:LEU:HD12	1:B:392:LEU:CD2	2.48	0.43
1:B:514:TRP:CD1	1:B:514:TRP:C	2.91	0.43
1:A:460:TRP:CD1	1:A:546:LEU:HD22	2.54	0.43
1:B:325:THR:HG22	1:B:370:PHE:CD2	2.54	0.43
1:B:364:ASN:HB3	1:B:367:ILE:HD12	2.00	0.42
1:A:403:ILE:CG2	1:A:404:VAL:N	2.82	0.42
1:A:365:PRO:HA	1:A:368:GLN:HB2	2.01	0.42
1:A:198:PRO:HG3	1:A:514:TRP:CH2	2.52	0.42
1:B:498:LEU:C	1:B:498:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:O	1:B:143:ILE:CG1	2.68	0.42
1:B:275:ILE:HD13	1:B:345:PRO:HD2	2.02	0.42
1:A:291:THR:HB	1:A:387:TYR:OH	2.19	0.41
1:A:242:GLN:OE1	1:A:242:GLN:N	2.53	0.41
1:A:278:ALA:HB1	1:A:283:ILE:HB	2.03	0.41
1:A:388:ILE:HD12	1:A:388:ILE:HA	1.94	0.41
1:B:433:LEU:O	1:B:437:THR:OG1	2.29	0.41
1:B:207:ILE:HG12	1:B:234:LEU:HD11	2.02	0.41
1:B:547:TYR:CG	1:B:548:ALA:N	2.88	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.94	0.41
1:B:444:ILE:HD13	1:B:444:ILE:HG21	1.67	0.41
1:B:504:PRO:HG3	1:B:533:ARG:HG3	2.03	0.41
1:B:504:PRO:O	1:B:507:SER:HB2	2.21	0.41
1:A:147:GLU:O	1:A:167:GLY:HA2	2.21	0.40
1:B:148:SER:O	1:B:167:GLY:HA3	2.21	0.40
1:A:307:THR:HG21	1:A:367:ILE:CD1	2.52	0.40
1:B:126:GLN:HE22	1:B:128:LEU:HD21	1.85	0.40
1:B:251:PHE:HB2	1:B:254:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	473/556 (85%)	448 (95%)	23 (5%)	2 (0%)	34 66
1	B	474/556 (85%)	436 (92%)	34 (7%)	4 (1%)	19 49
All	All	947/1112 (85%)	884 (93%)	57 (6%)	6 (1%)	25 56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	LYS
1	A	165	VAL
1	B	470	ASP
1	B	216	VAL
1	B	331	SER
1	B	458	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/486 (88%)	405 (95%)	21 (5%)	25	57
1	B	426/486 (88%)	402 (94%)	24 (6%)	21	51
All	All	852/972 (88%)	807 (95%)	45 (5%)	22	54

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	78	TYR
1	A	122	THR
1	A	165	VAL
1	A	183	SER
1	A	218	ILE
1	A	262	LEU
1	A	276	GLU
1	A	296	LEU
1	A	331	SER
1	A	338	LYS
1	A	347	GLN
1	A	385	SER
1	A	389	GLN
1	A	398	ILE
1	A	404	VAL
1	A	412	LYS
1	A	414	LYS

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Mol	Chain	Res	Type
1	A	427	SER
1	A	431	GLU
1	A	502	LEU
1	B	66	THR
1	B	90	SER
1	B	122	THR
1	B	125	GLN
1	B	132	THR
1	B	134	GLN
1	B	151	LEU
1	B	165	VAL
1	B	183	SER
1	B	257	LYS
1	B	261	SER
1	B	262	LEU
1	B	276	GLU
1	B	296	LEU
1	B	318	SER
1	B	347	GLN
1	B	385	SER
1	B	397	THR
1	B	398	ILE
1	B	404	VAL
1	B	412	LYS
1	B	427	SER
1	B	475	GLN
1	B	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	126	GLN
1	A	389	GLN
1	B	68	ASN
1	B	123	GLN
1	B	125	GLN
1	B	126	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	1.70	5 (29%)
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	2.36	5 (29%)
2	BMA	C	3	2	11,11,12	1.32	2 (18%)	15,15,17	1.77	4 (26%)
3	NAG	D	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	1.05	0
3	NAG	D	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.63	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BMA	C2-C3	2.46	1.56	1.52
2	C	1	NAG	O5-C1	-2.22	1.40	1.43
3	D	2	NAG	C1-C2	2.12	1.55	1.52
3	D	1	NAG	O5-C1	-2.04	1.40	1.43
2	C	3	BMA	C4-C5	2.01	1.57	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	O5-C1-C2	-6.42	101.15	111.29
2	C	3	BMA	C3-C4-C5	3.92	117.24	110.24
2	C	1	NAG	C3-C4-C5	-3.82	103.42	110.24
2	C	2	NAG	C2-N2-C7	3.81	128.33	122.90
2	C	2	NAG	C1-O5-C5	3.45	116.86	112.19
2	C	3	BMA	C2-C3-C4	2.98	116.06	110.89
3	D	2	NAG	C2-N2-C7	2.80	126.90	122.90
3	D	2	NAG	O5-C1-C2	-2.50	107.35	111.29
2	C	1	NAG	O6-C6-C5	-2.45	102.90	111.29
3	D	2	NAG	C1-C2-N2	2.43	114.64	110.49
2	C	3	BMA	O5-C1-C2	-2.42	107.03	110.77
2	C	1	NAG	O4-C4-C5	2.36	115.15	109.30
2	C	1	NAG	C4-C3-C2	2.35	114.46	111.02
2	C	2	NAG	O4-C4-C3	2.29	115.65	110.35
2	C	2	NAG	O6-C6-C5	-2.23	103.65	111.29
2	C	1	NAG	C1-C2-N2	2.22	114.27	110.49
3	D	2	NAG	O5-C5-C6	2.19	110.64	107.20
3	D	2	NAG	C1-O5-C5	2.10	115.04	112.19
2	C	3	BMA	O5-C5-C4	2.01	115.71	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
3	D	2	NAG	C3-C2-N2-C7

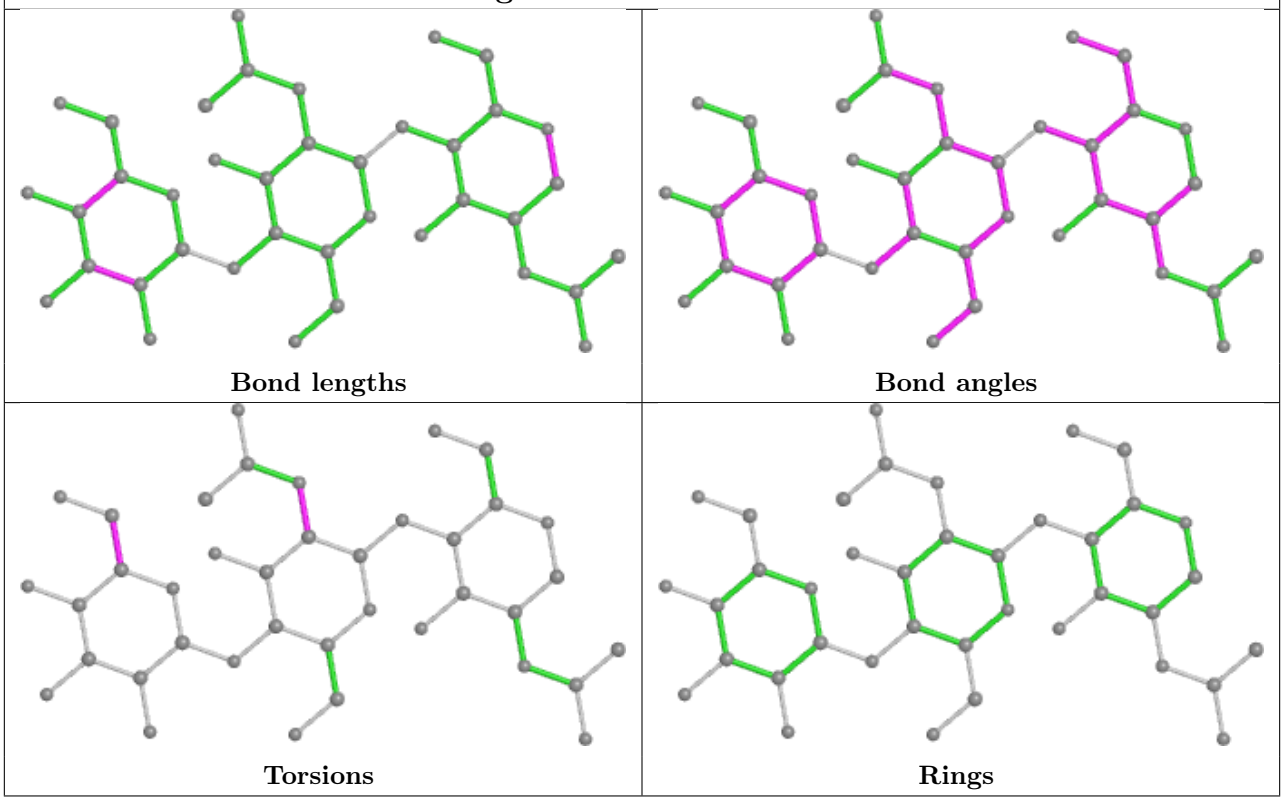
There are no ring outliers.

4 monomers are involved in 6 short contacts:

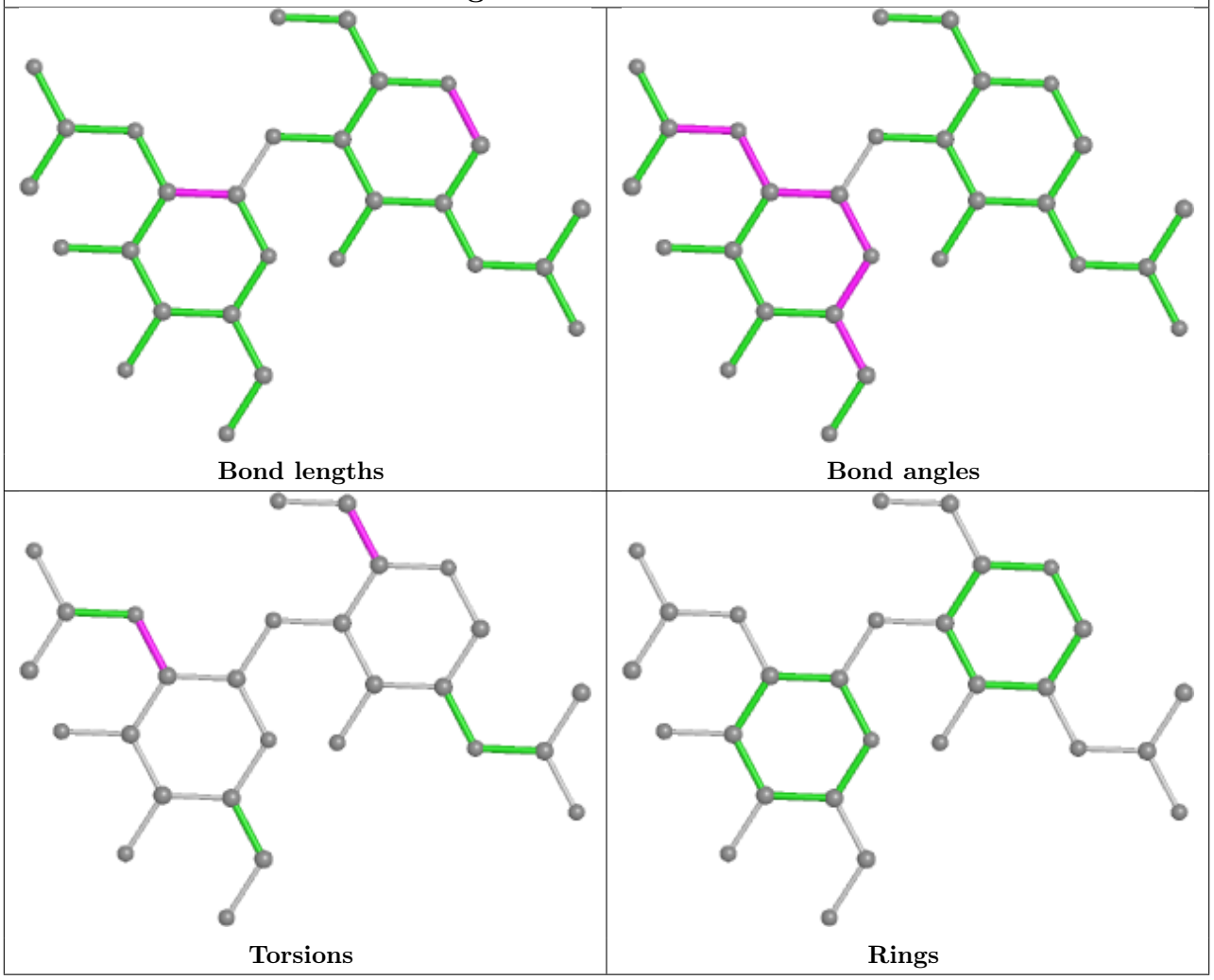
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	1	NAG	3	0
2	C	3	BMA	1	0
3	D	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CP6	A	562	-	17,18,18	1.77	5 (29%)	21,25,25	3.02	6 (28%)
5	NAG	B	559	1	14,14,15	1.33	1 (7%)	17,19,21	2.48	4 (23%)
4	NDG	A	560	-	14,14,15	1.27	2 (14%)	17,19,21	2.23	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	B	562	-	4,4,4	0.13	0	6,6,6	0.53	0
5	NAG	B	560	1	14,14,15	0.71	0	17,19,21	2.39	7 (41%)
4	NDG	B	561	-	14,14,15	1.33	1 (7%)	17,19,21	1.87	4 (23%)
5	NAG	A	561	1	14,14,15	1.35	2 (14%)	17,19,21	3.15	8 (47%)
6	CP6	B	563	-	17,18,18	1.95	4 (23%)	21,25,25	3.10	9 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CP6	A	562	-	-	2/2/6/6	0/2/2/2
5	NAG	B	559	1	-	2/6/23/26	0/1/1/1
4	NDG	A	560	-	-	0/6/23/26	0/1/1/1
5	NAG	B	560	1	-	1/6/23/26	0/1/1/1
4	NDG	B	561	-	-	2/6/23/26	0/1/1/1
5	NAG	A	561	1	-	2/6/23/26	0/1/1/1
6	CP6	B	563	-	-	1/2/6/6	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	563	CP6	C10-CL1	4.72	1.84	1.74
6	B	563	CP6	C5-N6	3.77	1.36	1.32
6	A	562	CP6	C5-N6	3.73	1.36	1.32
4	B	561	NDG	C1-C2	3.39	1.57	1.52
6	A	562	CP6	C10-CL1	3.35	1.81	1.74
5	A	561	NAG	C1-C2	3.00	1.56	1.52
4	A	560	NDG	C1-C2	3.00	1.56	1.52
5	B	559	NAG	C1-C2	2.54	1.56	1.52
6	A	562	CP6	C11-C10	2.39	1.42	1.38
6	B	563	CP6	C11-C10	2.31	1.42	1.38
4	A	560	NDG	C3-C2	2.25	1.57	1.52
6	B	563	CP6	C12-C11	2.16	1.41	1.36
6	A	562	CP6	C12-C11	2.16	1.41	1.36
6	A	562	CP6	C8-C9	2.09	1.41	1.36
5	A	561	NAG	C2-N2	2.05	1.49	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	562	CP6	C2-N6-C5	8.90	123.66	116.24
6	B	563	CP6	C4-C5-N6	-8.08	116.57	122.44
6	B	563	CP6	C2-N6-C5	7.11	122.17	116.24
5	A	561	NAG	C2-N2-C7	6.67	132.40	122.90
6	A	562	CP6	C4-C5-N6	-6.33	117.84	122.44
5	B	560	NAG	C1-O5-C5	6.11	120.47	112.19
6	A	562	CP6	C5-C4-C3	-5.85	118.11	123.34
5	A	561	NAG	O5-C1-C2	5.53	120.02	111.29
5	A	561	NAG	C1-O5-C5	5.47	119.60	112.19
5	B	559	NAG	C4-C3-C2	5.47	119.03	111.02
4	A	560	NDG	C1-O5-C5	5.29	119.36	112.19
5	B	559	NAG	C1-O5-C5	4.98	118.95	112.19
5	A	561	NAG	O5-C5-C6	4.92	114.92	107.20
4	B	561	NDG	C2-N2-C7	4.83	129.77	122.90
6	B	563	CP6	C8-C9-C10	4.67	124.64	119.21
5	B	559	NAG	C2-N2-C7	4.52	129.34	122.90
6	A	562	CP6	N6-C2-N1	-4.14	118.92	125.42
6	B	563	CP6	C11-C10-CL1	4.02	125.63	119.35
5	B	560	NAG	O5-C5-C6	-3.99	100.95	107.20
4	A	560	NDG	O5-C1-C2	3.82	117.32	111.29
5	B	560	NAG	C4-C3-C2	3.77	116.55	111.02
5	B	559	NAG	C3-C4-C5	3.45	116.39	110.24
4	B	561	NDG	C1-O5-C5	3.31	116.67	112.19
4	A	560	NDG	C1-C2-N2	-3.24	104.96	110.49
5	A	561	NAG	C3-C4-C5	-3.02	104.86	110.24
6	B	563	CP6	C11-C10-C9	-2.83	117.57	121.24
4	B	561	NDG	O5-C1-C2	2.75	115.63	111.29
6	B	563	CP6	C5-C4-C3	-2.74	120.89	123.34
6	B	563	CP6	N6-C2-N1	-2.57	121.39	125.42
4	B	561	NDG	O5-C5-C6	2.51	111.14	107.20
5	A	561	NAG	O7-C7-N2	2.47	126.50	121.95
4	A	560	NDG	O7-C7-N2	2.42	126.41	121.95
5	B	560	NAG	C2-N2-C7	-2.41	119.47	122.90
6	B	563	CP6	C15-C5-N6	2.29	121.66	116.67
5	B	560	NAG	O4-C4-C5	2.28	114.97	109.30
5	B	560	NAG	O4-C4-C3	-2.25	105.15	110.35
5	A	561	NAG	O4-C4-C5	2.24	114.86	109.30
4	A	560	NDG	O5-C5-C6	2.22	110.69	107.20
6	A	562	CP6	N14-C2-N6	2.17	120.62	117.25
6	B	563	CP6	C9-C8-C7	-2.10	117.57	120.82
5	B	560	NAG	C3-C4-C5	2.09	113.97	110.24
6	A	562	CP6	N14-C2-N1	2.06	120.45	117.25
5	A	561	NAG	O4-C4-C3	2.04	115.07	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	562	CP6	C16-C15-C5-C4
6	B	563	CP6	C16-C15-C5-C4
5	B	559	NAG	C4-C5-C6-O6
5	A	561	NAG	O5-C5-C6-O6
5	B	559	NAG	O5-C5-C6-O6
5	A	561	NAG	C4-C5-C6-O6
4	B	561	NDG	C1-C2-N2-C7
6	A	562	CP6	C16-C15-C5-N6
4	B	561	NDG	C3-C2-N2-C7
5	B	560	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	562	CP6	8	0
6	B	563	CP6	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	479/556 (86%)	-0.46	3 (0%)	89	86	36, 50, 77, 92	0
1	B	480/556 (86%)	-0.40	3 (0%)	89	86	38, 54, 74, 88	0
All	All	959/1112 (86%)	-0.43	6 (0%)	89	86	36, 52, 75, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	ASP	4.9
1	A	311	SER	4.6
1	B	311	SER	3.7
1	A	317	ASP	3.3
1	A	122	THR	2.9
1	B	414	LYS	2.8

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	C	3	11/12	0.55	0.39	100,104,105,106	0
3	NAG	D	2	14/15	0.82	0.49	91,95,99,99	0
3	NAG	D	1	14/15	0.91	0.24	63,72,75,83	0

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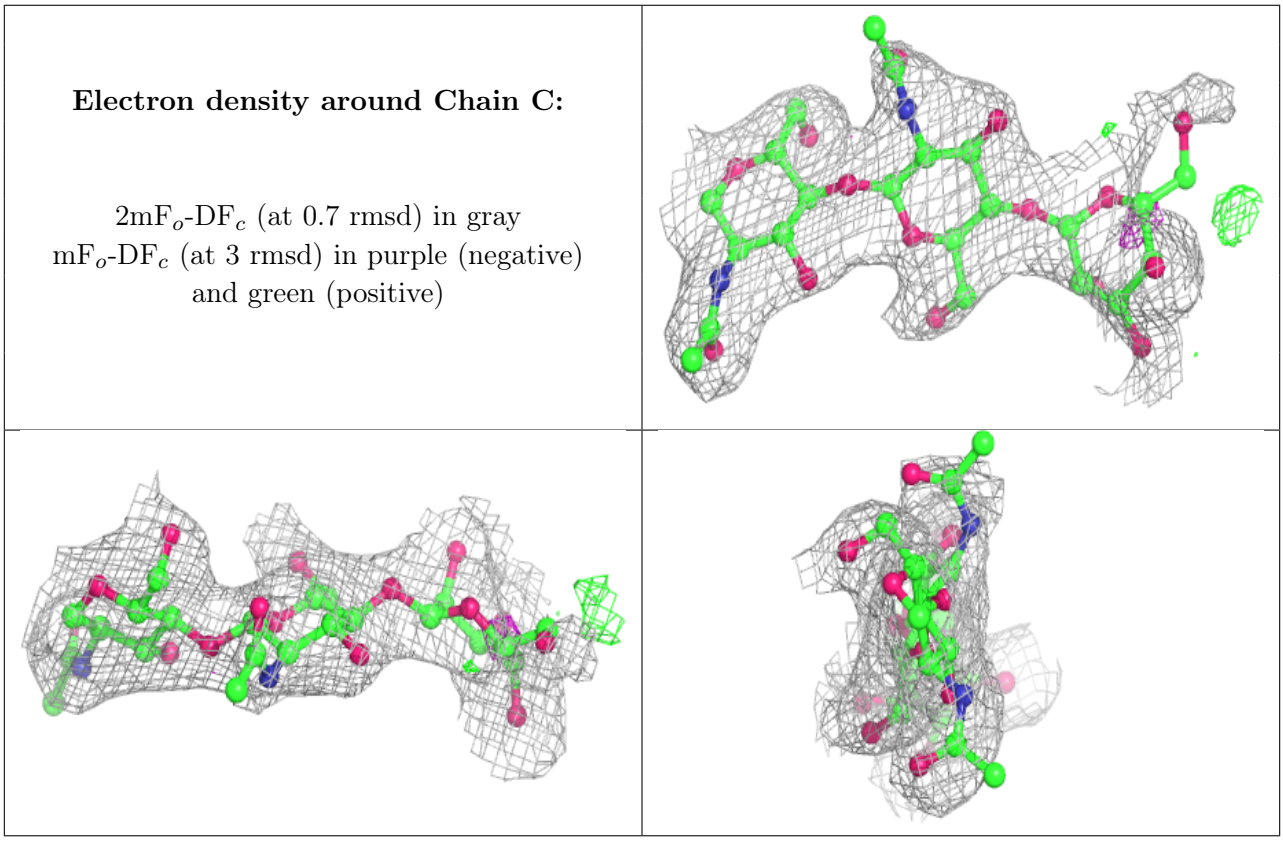
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.92	0.34	77,83,88,95	0
2	NAG	C	1	14/15	0.96	0.23	49,55,59,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

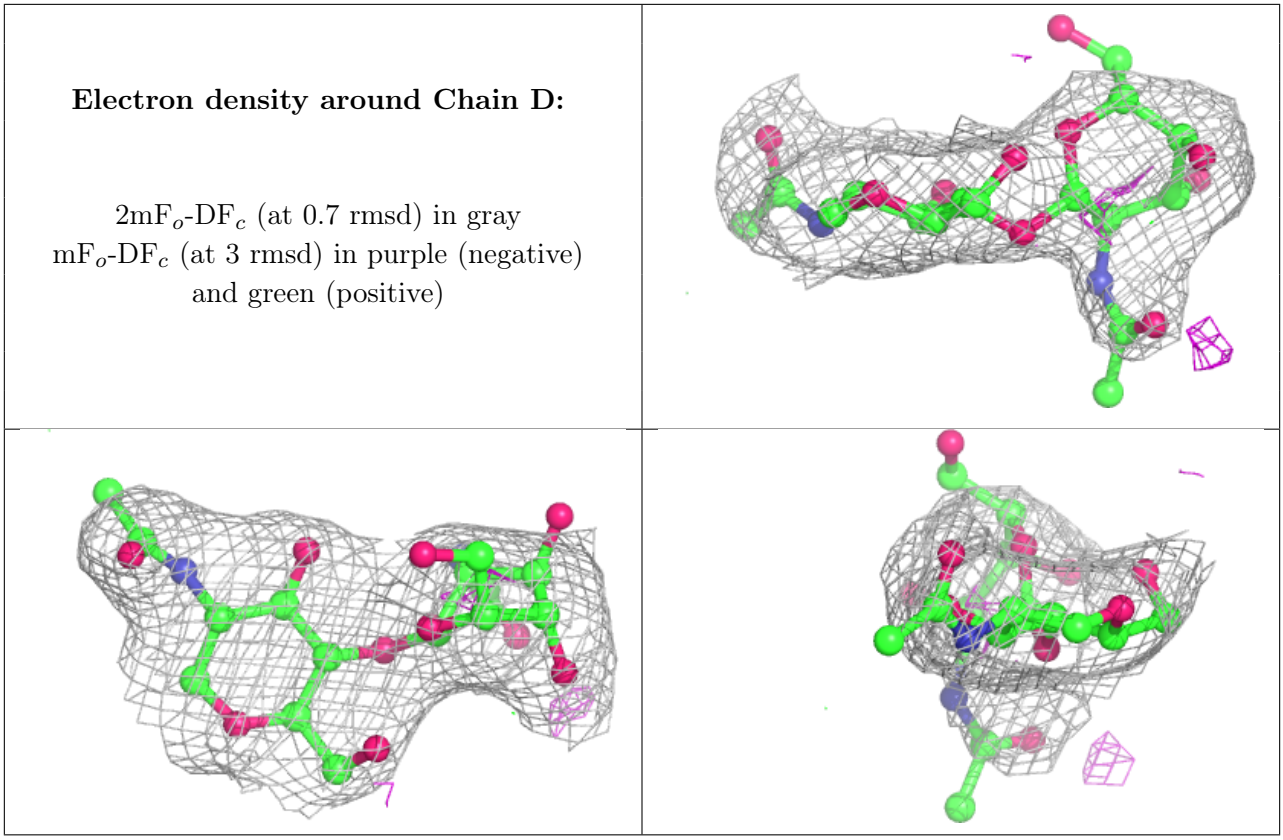
Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	561	14/15	0.66	0.50	91,99,100,101	0
5	NAG	B	559	14/15	0.78	0.36	75,85,90,91	0
4	NDG	A	560	14/15	0.81	0.32	81,89,91,91	0
6	CP6	B	563	17/17	0.81	0.25	51,62,81,86	0
4	NDG	B	561	14/15	0.82	0.45	89,95,103,104	0
6	CP6	A	562	17/17	0.85	0.24	68,75,97,102	0
5	NAG	B	560	14/15	0.88	0.32	78,83,88,90	0
7	SO4	B	562	5/5	0.97	0.09	69,71,72,74	0

6.5 Other polymers

There are no such residues in this entry.